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Calculation of Muon Depth Distributions in Thin Film Single Crystals

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Abstract

To investigate the effects of sample crystallinity and the consequent channeling on the stopping distribution of low energy muons, we compare the results of the well-known binary-collision-approximation code(BCA): TRIM to results from MARLOWE from Oak Ridge National Laboratory, and those of a code which we have written and given the acronym MUSCLE. TRIM assumes an amorphous stopping medium. MARLOWE is also a BCA code, but treats the stopping medium as crystalline. MUSCLE uses a molecular dynamics approach and should be even more accurate. For the results shown here we use bcc Fe. TRIM, MARLOWE, and MUSCLE are Monte-Carlo codes. We find that the average penetration depths are similar, but that the detailed shapes of the penetration distributions are quite different. When the dependence of the interpretation of experiments depends on the relative probabilities of penetration depth, a use of code which includes the effects of crystallinity is recommended.

Keywords: Muon transport, Thin Crystalline Films, muSR
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1. Introduction

With the advent of muon beams capable of stopping in thin layers of crystalline material[1] it becomes important to know the depth distribution of these muons in order to properly interpret muon spin rotation, (μSR), experiments. For example, in the direct determination of the penetration depth of a superconductor by Kiefl et al.[2], this distribution is used and its uncertainty is the largest uncertainty of the measurements. The program named TRIM is often used by some researchers [3]. TRIM simulates the passage of ions through samples using the Binary Collision Approximation (BCA) method. However, TRIM assumes that the stopping material is amorphous and so does not treat effects due to crystallinity. For crystalline structure, channeling of particles (constrained motion along crystallographic directions) can allow anomalously deep penetration for some muons which in turn will affect their spatial stopping-distribution. In order to investigate this issue, we have used MARLOWE [4], another BCA program, but one which does include the effects of crystallinity. This program is available from ORNL. We have also written a collection of programs called MUSCLE (MUonS Cascade at Low Energy) that include an approximation scheme to detect channeling of muons in a crystal and a molecular dynamics model that should give an even better estimate of the channeling process. We have chosen to work with iron, a bcc crystal, for all demonstrations. TRIM, MARLOWE, and MUSCLE are Monte-Carlo codes.

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2. TRIM Calculations

For subsequent comparison we ran simulations of muons stopping in iron using the code TRIM. The results for 500 eV, 1.5 keV, and 5 keV are shown in Fig. 1. All results are normalized so that the sum over the curves with a 1 Å step size is one. Also to facilitate comparison all the graphs have a maximum on the penetration, x, axis of 600 Å.

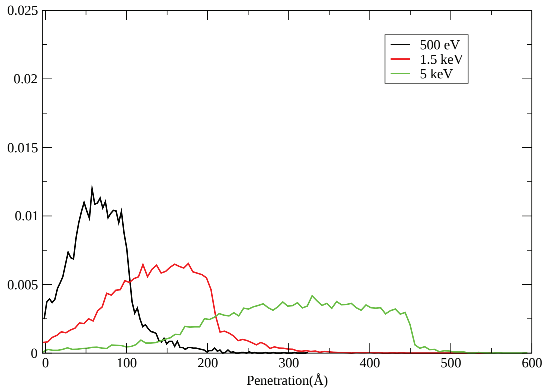

Figure 1: Stopping distributions produced from TRIM for 500 eV, 1.5 keV, and 5 keV muons.and varying beam divergence. The stopping material is Fe of arbitrary lateral size.

3. Crystal Structure

As a reasonable example we chose to consider the bcc system of iron. We assumed that the muons would be incident more or less parallel to the [100] direction. If the conventional cubic structure is aligned so that the Fe ions on the face of the cube are along the x and y directions, then diamond shaped channels are formed between two of the face ions and two of the body-centered ions. Through these channels the muons can be constrained and for the most part do not experience large angle scattering.

4. MARLOWE Simulations

MARLOWE is a BCA program that takes account of multiple collisions. MARLOWE solves the scattering integral using a 32-point Gauss-Mehler procedure. This comes at the expense of increased computation time, but should yield more accurate results [5].

The results for 500 eV, 1.5 keV, and 5 keV show indications of channeling. Results for various divergences show very little change at 500 eV, the beginnings of marked differences for 1.5 keV, and perhaps even surprising differences for 5 keV.

5. Molecular Dynamics Simulations

Molecular Dynamics (MD) simulations take into account the simultaneous scattering from a number of neighbor atoms [6]. Thus, these may also provide a better estimation of channeling and transmission out of the sample, and some researchers prefer this model for their ion beam experiments and simulations [7]. For MUSCLE, we have written a basic molecular dynamics program for muon beams. Our program uses the recoil interaction approximation method [6] where we ignore the interactions between target atoms and only keep track of the muon and its surrounding atoms at each time step to reduce the computation time. The force on the projectile is given by the summation of all the forces from the neighbors, and the forces are derivable from a potential.

$$M_i \frac{d^2 \vec{r_i}(t)}{dt^2} = \sum_{j=1}^{N} \vec{F_{ij}} = \vec{F_i}(\vec{r_i}(t)) = -\sum_{j \neq j} \nabla V_{ij}(\vec{r_{ij}})$$

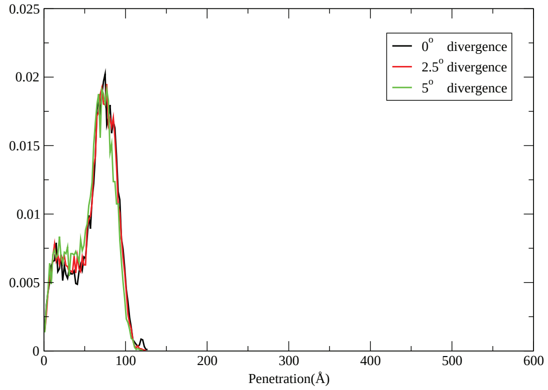

Figure 2: Stopping distributions produced from MARLOWE for 500 eV muons and varying beam divergence. The stopping material is crystalline Fe of arbitrary lateral size. The muons are incident parallel to the [100] direction of the conventional unit cell of this bcc material.

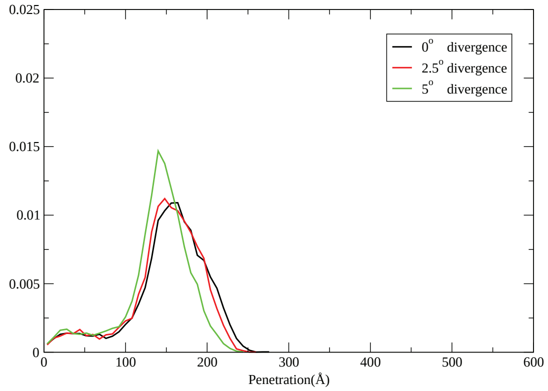

Figure 3: Stopping distributions produced from MARLOWE for 1.5 keV muons and varying beam divergence. The stopping material is crystalline Fe of arbitrary lateral size. The muons are incident parallel to the [100] direction of the conventional unit cell of this bcc material.

where M_i stands for the mass of the projectile, and N is the total number of neighbors at a given instant of time. The central difference method is used for numerical integration. The time step is chosen so that the fastest projectile will not traverse more than 5% of the distance equivalent to the lattice constant, $\triangle t = 0.05\, d\, \sqrt{M/2T_m}$, where T_m represents the kinetic energy of the projectile with mass M, and d is the lattice constant. The Born-Mayer potential function is used:

$$V(\vec{r}) = A_{BM}\, e^{-\frac{|\vec{r}|}{a_{BM}}}$$

where A_{BM} is an energy parameter and a_{BM} is the screening length.

6. Results, Comments and Conclusions

The average penetration depths for 500 eV muons in Fe using TRIM, MARLOWE, and MUSCLE are respectively: 70.49, 62.4, and 68.85 Å. The average ranges, overall, are quite similar, but by comparing the figures one can see the the shapes of the distributions are quite different. The MARLOWE results differ from those of TRIM and MUSCLE by having a low range plateau below the peak in the distributions. At 5 keV MARLOWE has a much smaller low energy plateau and has distribution reaching to 500 Å. The striking reduction in penetration and narrowing of the distribution seen upon varying the beam divergence for 5 keV muons needs to be explored further.

If one is using the stopping distributions in the analysis of experiments and the medium is crystalline, the use of codes which include the effects of this crystallinity is recommended.

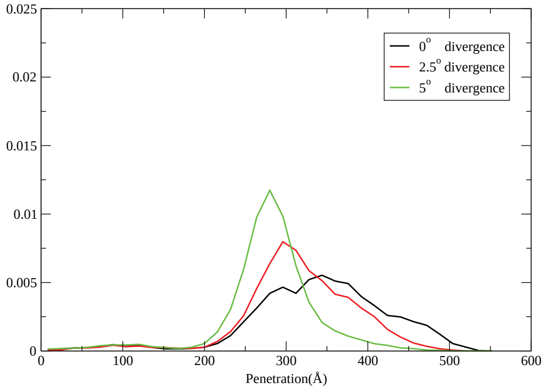

Figure 4: Stopping distributions produced from MARLOWE for 5 keV muons and varying beam divergence. The stopping material is crystalline Fe of arbitrary lateral size. The muons are incident parallel to the [100] direction of the conventional unit cell of this bcc material.

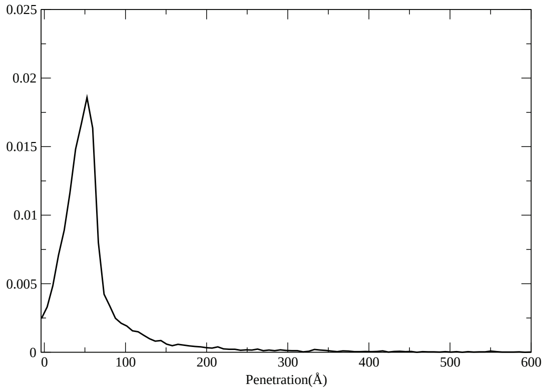

Figure 5: Stopping distributions produced from MUSCLE with 500 eV muons. The stopping material is crystalline Fe of arbitrary lateral size. The muons are incident parallel to the [100] direction of the conventional unit cell of this bcc material.

References

[1] E. Morenzoni, H. G. T. Prokscha, H. P. Weber, E. M. Forgan, T. J. Jackson, H. Luetkens, C. Niedermayer, M. Pleines, M. Birke, A. Hofer, J. Litterst, T. Riseman, G. Schatz, Low-energy μSR at PSI: present and future, Physica B 289-290 (2000) 653–657.

[2] R. F. Kiefl, M. D. Hossain, B. M. Wojek, S. R. Dunsiger, G. D. Morris, T. Prokscha, Z. Salman, J. Baglo, D. A. Bonn, R. Liang, W. N. Hardy, A. Suter, E. Morenzoni, Direct measurement of the London penetration depth in $YBa_2Cu_3O_{6.92}$ using low-energy μSR, Physical Review B 81 (2010) 180502.

[3] M. Dubman, T. Shiroka, H. Luetkens, M. Rothermal, F. J. Litterst, E. Morenzoni, A. S. adn D. Spemann, P. Esquinazi, A. Setzer, T. Butz, Low energy μSR and SQUID evidence of magnetism in highly oriented pyrolytic graphite, Journal of Magnetism and Magnetic Materials 322 (2009) 1228.

[4] M. T. Robinson, Computer simulation studies of high-energy collision cascades, Phys. Rev. B 67 (92) 396.

[5] W. Eckstein, Computer Simulation of Ion-Solid Interactions, Spring-Verlag, 1991.

[6] K. Nordlund, Molecular dynamics for ion beam analysis, Nuclear Instruments and Methods in Physics Resear B 266 (2008) 1886.

[7] K. Nordlund, Molecular dynamics simulation of ion ranges in the 1 - 100 kev energy range, Comp. Mat. Sci. 3 (1995) 448.